

“Critical” phonons of the supercritical Frenkel-Kontorova model: renormalization bifurcation diagrams

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The phonon modes of the Frenkel-Kontorova model are studied both at the pinning transition as well as in the pinned (cantorus) phase. We focus on the minimal frequency of the phonon spectrum and the corresponding generalized eigenfunction. Using an exact decimation scheme, the eigenfunctions are shown to have nontrivial scaling properties not only at the pinning transition point but also in the cantorus regime. Therefore the phonons defy localization and remain *critical* even where the associated area-preserving map has a positive Lyapunov exponent. In this region, the critical scaling properties vary continuously and are described by a line of renormalization limit cycles. Interesting renormalization bifurcation diagrams are obtained by monitoring the cycles as the parameters of the system are varied from an integrable case to the anti-integrable limit. Both of these limits are described by a trivial decimation fixed point. Very surprisingly we find additional special parameter values in the cantorus regime where the renormalization limit cycle degenerates into the above trivial fixed point. At these “degeneracy points” the *phonon* hull is represented by an infinite series of step functions. This novel behavior persists in the extended version of the model containing two harmonics. Additional richnesses of this extended model are the one to two-hole transition line, characterized by a divergence in the renormalization cycles, nonexponentially localized phonons, and the preservation of critical behavior all the way upto the anti-integrable limit.

I. INTRODUCTION

The Frenkel-Kontorova (FK) model is one of the simplest prototypes for theoretical studies on incommensurate structures in solid-state physics [4,7,13]. The model consists of an infinite one-dimensional chain of balls in an external sinusoidal potential with an elastic interaction between nearest neighbors. If the mean distance between consecutive balls is not in rational proportion to the periodicity of the sinusoidal potential, the corresponding state is called incommensurate. Incommensurate structures appear in many physical systems such as quasicrystals, two-dimensional electron systems, magnetic superlattices, and charge-density waves.

Because of the well-known connection to the area-preserving standard map, the FK model is important also from the nonlinear-dynamics point of view. An incommensurate ground state of the FK model corresponds either to an invariant circle or a cantorus (invariant Cantor set) for the standard map. In the Kolmogorov-Arnol’d-Moser (KAM) phase, a configuration associated with a smooth circle can be described by an analytic hull function which maps a rigid rotation orbit to the configuration. On the other hand, a cantorus corresponds to a purely discrete hull function representable as a convergent series of step functions [6]. Physically, a state with an analytic hull function is free to slide whereas a discrete hull function implies a non-zero minimum force (or field) required for depinning. The pinning transition corresponding to the breakup of an invariant circle is usually referred as the transition by breaking of analyticity (TBA).

The linear excitation or the phonon modes of the FK model describing the physical stability of the states are affected in an important way by the TBA. In the KAM phase and at the TBA, it is possible to find a translational mode with zero frequency (phason mode) supporting collective transport. The corresponding generalized phonon eigenfunctions are “extended” (quasiperiodic) in the KAM phase and “critical” (neither extended nor localized) with non-trivial scaling properties at the TBA. However, not much has been known about the eigenfunctions in the cantorus regime where the frequencies of phonons are bounded away from zero. In a related quantum problem, describing an electron in a quasiperiodic potential, a similar transition results in localized eigenfunctions [20]. On the other hand, the absence of localization has been proven for a quasiperiodic potential taking a finite number of discrete values [14]. Although the potential seen by the phonons is purely discrete in the cantorus regime, the potential still takes an infinite number of distinct values which leaves the question on the nature of the eigenfunctions open. There are recent speculations by Burkov et al. [12] on the possibility of having critical phonon modes at band edges of the phonon spectrum. However, in their numerical study, where the localiza-

tion character is inferred by computing the participation ratio, it is rather difficult to make definite predictions.

A great deal of effort has been put on studying the non-trivial scale invariance observed at the TBA [13,15,16,23]. MacKay [22] has adjusted his previous renormalization theory for the critical invariant circles to explain many scaling exponents in the neighborhood of the transition. However, it has not been clear how to formulate the scaling theory in the supercritical cantorus region where many relevant quantities like the actions or phase space scaling constants diverge in renormalizing [21]. Sneddon et al. [26] took a step in this direction by proposing a renormalization theory of the pinning threshold in the case of infinite viscosity. Working in the Fourier basis, they found three-term harmonic expansions for both the TBA renormalization fixed point and the new dynamic-threshold fixed point characterizing the depinning transition at a critical field in the supercritical regime. The latter fixed point corresponded to vanishing elastic constants.

In this paper, an exact decimation approach [17,19,20] is used to study phonons in the FK model both at the TBA and beyond the transition. We show that the minimal frequency phonon mode remains critical throughout the cantorus regime. Furthermore, the scaling properties of the corresponding generalized eigenfunctions vary continuously and are characterized by a line of limit cycles of the renormalization equations. We numerically obtain a full bifurcation diagram of these cycles as the system parameter is varied upto the anti-integrable limit where the elastic interaction disappears. The limit cycle degenerates to a trivial fixed point at the anti-integrable limit and at an infinite sequence of other parameter values approaching the TBA from above. At this sequence of points, the phonon eigenfunctions are represented by infinite series of step functions and hence provide novel behavior in the study of systems with competing periodicities. The degeneracy points persist in the FK model with two harmonics and hence are believed to be generic in one-parameter families of similar models.

We also investigate the scaling properties of one to two-hole transition [10] for cantori in a two-harmonic model. Using a multi-precision software package [11], we show that the transition is signalled by a divergence in one member of the limit cycle of the renormalization trajectory. However, the finite members of the limit cycle vary continuously along the transition line in the two-parameter space. This transition line is distinguished from the rest of the cantorus phase by the fact that the phonon eigenfunctions vanish asymptotically. However, the localization is not exponential as suggested by vanishing of the Lyapunov exponent. Another new feature existing only for a two-hole cantorus is the non-trivial anti-integrable limit for phonons, i.e. the phonons remain critical all the way upto the anti-integrable limit.

The FK model, its relation to the standard map and

the phonon modes describing the physical stability of the FK model are briefly reviewed in Section II. Section III explains the decimation method which has been previously applied to investigate the critical invariant circles in dissipative systems [17] and the self-similar wave functions in tight binding models [19,20]. In Section IV we give an account of the numerical methods used in our study. The results of applying the decimation method to the FK model are reported in Section V. Analogous results on the extended FK model with two harmonics are found in Section VI. The main emphasis there is on the one to two-hole transition. The results and some open problems are discussed in Section VII. An appendix contains a detailed discussion on what happens to the phonons approaching the anti-integrable limit.

II. GENERALITIES

This section is about the FK model, terminology and basic results of Aubry's [4,7] theory.

A configuration of the FK model is defined as the sequence x_i , $i \in \mathbb{Z}$, where x_i gives the position of the i th ball. The energy of the configuration is given by

$$W = \sum_i v(x_i, x_{i+1}), \quad (1)$$

where v is the generating function

$$v(x_i, x_{i+1}) = \frac{1}{2}(x_{i+1} - x_i - a)^2 + V(x_i), \quad (2)$$

$$V(x) = \frac{k}{4\pi^2} \cos(2\pi x). \quad (3)$$

Because the external potential part V of the energy has the period unity, two configurations x and \tilde{x} can be identified if there exist $m, n \in \mathbb{Z}$ such that the transformation $(T_{mn}x)_i = x_{i+m} - n$ maps x on \tilde{x} . An equilibrium state with $\partial W / \partial x_i = 0$ for all $i \in \mathbb{Z}$ is obtained by iterating the area-preserving standard map

$$(x_{i+1}, y_{i+1}) = F(x_i, y_i) = (x_i + y_{i+1}, y_i + V'(x_i)), \quad (4)$$

where $y_i = x_i - x_{i-1}$.

A *minimum energy (m.e.) state* is defined as a configuration x such that the energy for all other configurations which agree with x outside a finite range of i is greater than or equal to the energy of x . Every m.e. state is rotationally ordered [7] which implies the existence of the mean spacing of the balls given by the rotation number

$$\sigma = \lim_{N \rightarrow \infty} \frac{x_N - x_0}{N}. \quad (5)$$

Incommensurate states correspond to irrational values of σ .

One is usually interested in *recurrent* m.e. states which are called *ground states* by Aubry [4]. There exists a

closed non-empty set of recurrent m.e. states of every mean spacing $\sigma \in R$. If σ is irrational, this set corresponds either to an invariant circle or a cantor set around the cylinder obtained by identifying x and $x + 1$. In other words, the FK model can have an infinite number of ground states all corresponding to the same invariant circle or cantor set of the standard map. An invariant circle can be described by a unique strictly increasing continuous *hull function* $g : R \rightarrow R$ so that

$$x_i = g(i\sigma + \phi), \quad g(\theta + 1) = g(\theta) + 1, \quad (6)$$

where by varying the phase ϕ one can choose the ground state one wants. There is a similar representation for a cantor set in terms of either the left- or right-continuous extension of a unique non-decreasing discontinuous hull function.

The *physical* ground states are obtained by minimizing the energy per ball over σ . For the FK model, the parameter a can be tuned for each k so that the physical ground states have a desired mean spacing.

The equation describing the physical stability of the ball configurations in the FK model is obtained by linearizing the dynamics $d^2x_i/dt^2 = -\partial W/\partial x_i$ about an equilibrium configuration. The resulting equation for the small displacements ξ_i is

$$\frac{d^2\xi_i}{dt^2} = -\frac{\partial^2 W}{\partial x_i \partial x_j} \xi_j \quad (7)$$

which can be written in the compact way $d^2\xi/dt^2 = -D^2W\xi$. The *phonon modes* are solutions of the form $\xi(t) = \exp(i\omega t)\psi$, where the (generalized) eigenvector ψ of the operator D^2W satisfies the equation

$$\psi_{i+1} + \psi_{i-1} - [2 + V''(x_i)]\psi_i = -\omega^2\psi_i. \quad (8)$$

The spectrum of D^2W , given in terms of the squares of phonon frequencies ω^2 , relates in an important way to the properties of the ground states of the FK model. First, it can be proven that the spectrum of D^2W does not depend on the phase of an incommensurate ground state in the FK model [6]. For an invariant circle, the infimum E_{min} of the spectrum is zero whereas for a uniformly hyperbolic cantor set $E_{min} > 0$ [8]. In general, the configurations with $E_{min} > 0$ are physically at least metastable. Moreover, uniform hyperbolicity implies structural stability, i.e. there cannot be any bifurcations of the cantor set at the corresponding parameter values. However, the cantor set can lose uniform hyperbolicity at a bifurcation where $E_{min} = 0$. Such bifurcations appear in extended versions of the FK model containing two or more harmonics [9,10,18,24].

III. PHONON DECIMATION

The phonon equation (8) can be interpreted as a discrete Schrödinger equation for the “wave function” ψ_i in

the quasiperiodic potential $2 + V''(g(i\sigma + \phi))$. Similar quasiperiodic linear-difference equations appear in many other nonlinear dynamics and solid state problems. We have developed a decimation method to deal with such equations [17,19,20]. The main advantage of the method is that the scaling properties of solutions can be described by bounded decimation functions. The decimation strategy is determined by the underlying “frequency” σ . Our decimation can be implemented for any irrational σ by choosing an arbitrary path in the Farey tree [19]. However, in this paper we will restrict ourselves to one of the noble rotation numbers, namely, $\sigma = \gamma^{-2}$, where $\gamma = \frac{1}{2}(1 + \sqrt{5})$ is the golden ratio.

In the decimation scheme, all other lattice sites except those labelled by the Fibonacci numbers F_n , $F_{n+1} = F_n + F_{n-1}$ ($F_0 = 0, F_1 = 1$), are decimated out beginning from an arbitrary initial site i . At the n^{th} step, the decimated phonon equation has the form

$$f_n(i)\psi(i + F_{n+1}) = \psi(i + F_n) + e_n(i)\psi(i). \quad (9)$$

The phonon frequency is simply a parameter in this decimation equation which therefore should not be considered as an eigenvalue problem. Using the additive property of the Fibonacci numbers, straightforward manipulations give the following exact recursion relations for the decimation functions e_n and f_n :

$$e_{n+1}(i) = -\frac{Ae_n(i)}{1 + Af_n(i)} \quad (10)$$

$$f_{n+1}(i) = \frac{f_{n-1}(i + F_n)f_n(i + F_n)}{1 + Af_n(i)} \quad (11)$$

$$A = e_{n-1}(i + F_n) + f_{n-1}(i + F_n)e_n(i + F_n).$$

The above recursion relations can be iterated numerically for an arbitrary number of decimation steps provided the phonon frequency ω and the sequence x_i , which set the initial functions $e_2(i)$ and $f_2(i)$, can be calculated with arbitrary precision.

There are a number of reasons why the iteration of the recursion relations (10-11) is superior to the direct iteration of the phonon equation (8):

- 1) Often the iteration of the recursion relations is numerically more stable than that of Eq. (8).
- 2) The possible self-similarity observed by monitoring the behaviour of ψ_i over the range $i \in [-F_n, F_n]$ with increasing n can be captured by a simple asymptotic limit cycle for the decimation functions e_n and f_n .
- 3) An unknown or inaccurate parameter in the equation (9) and the asymptotic limit cycle can be simultaneously determined self-consistently (see the next section for further details). In other words, the decimation equations themselves provide a new method to compute e.g. eigenvalues or phase boundaries up to machine precision.

The decimation scheme can also be used in describing the self-similar fluctuations of exponentially localized

modes. Here the localized eigenfunction is written as $\psi_i = e^{-\gamma|i|}\eta_i$ which results in the following equation for η_i :

$$e^{-\gamma}\eta_{i+1} + e^{\gamma}\eta_{i-1} - [2 + V''(x_i)]\eta_i = -\omega^2\eta_i \quad (12)$$

The above equation can be studied using the decimation scheme with the inverse localization length γ being an additional parameter. Again γ can be determined self-consistently along with the limit cycle. [2]

Although the above scheme with a discrete lattice index i is sufficient for the present purpose, we would like to point out that an analogous form of the recursion relations in terms of a continuous variable is needed if one wants to solve renormalization limit cycles by the Newton method [19,20].

IV. NUMERICAL METHODS

In this paper, the properties of the solutions to Eq. (8) are studied at the minimal frequency $\omega = \sqrt{E_{min}}$. In the KAM phase, the ground state configurations of the model exhibit a zero frequency phonon. In this case, the corresponding eigenfunction can be determined very accurately. At the TBA, the precision in obtaining the asymptotic scaling properties is limited by the precision of the critical k value and the sequence x_i . On the other hand, the iteration of the decimation equations for an arbitrary value of the nonlinearity parameter k in the cantorus regime is mainly limited by the precision of the phonon frequency. However, as pointed out in the previous section, the existence of asymptotic limit cycles for the decimation functions can be used to obtain the frequency to high precision so that the remaining source of numerical error is the inaccuracy of the ball positions. This error can be made very small by approximating a ground state with very long orbit.

There are essentially two steps involved in obtaining the scaling properties of the phonon eigenmodes. The first step is to obtain an estimate for the minimal frequency of the phonon spectrum using an orbit of moderate size (e.g. 610) in the diagonalization procedure. The frequency estimate has to be precise enough in order to allow so many decimation steps that the asymptotic cycle is already approached. Usually the diagonalization procedure is the most CPU time consuming part in the numerical calculations. The second part is to approximate the cantorus with a very long orbit (e.g. of the length 46368) and to improve the frequency estimate to very high precision so that the recursion relations (10-11) can be iterated many times to obtain the asymptotic cycle with several significant digits.

We follow Baesens and MacKay (see Appendix A of ref. [10]) in calculating an initial estimate for E_{min} and the sequence x_i for the decimation equation (8). An invariant

circle or a cantorus of rotation number γ^{-2} is approximated by periodic orbits of rotation numbers F_{n-2}/F_n . It is sufficient to consider symmetric periodic orbits which fall into four classes [10]: 1) even period with $x_0 = 0$, 2) even period with $x_0 = -x_1$, 3) odd period with $x_0 = 0$, and 4) odd period with $x_0 = 1/2$. These classes are useful in obtaining initial conditions for the iteration of Eq. (8) as the phonon modes in each class are either symmetric or antisymmetric [10]. In the KAM phase and at the TBA, the invariant circle describing the ball configurations can be approximated by any of the above four classes. However, a cantorus can be approximated only by class-2 (or class-4 if the cantorus has only one hole) orbits. The classes 1 and 3 (and 4 in the region of two holes, see section VI) give some homoclinics in addition to the cantorus so E_{min} can be different for them. Baesens and MacKay explain how to obtain the orbit Lyapunov exponent or the residue needed in locating the TBA and the one to two-hole transition on the parameter axis. It should be noted that in the cantorus phase, the standard map has a positive Lyapunov exponent which near anti-integrable limit exhibits a logarithmic divergence with the nonlinearity parameter k .

One of our main tasks was to decide on whether the eigenfunctions were exponentially localized or not. Thouless has derived a formula for the inverse localization length [25]. However, in practice the estimates obtained with this formula remain rather crude as it requires considering differences between all eigenvalues. Initially, we carried out the decimation varying the value of the inverse localization length γ but we found that only $\gamma = 0$ showed convergence towards a non-trivial asymptotic p -cycle for the decimation functions at $\omega = \sqrt{E_{min}}$. Assuming $\gamma = 0$, the value of E_{min} was then sequentially improved with the secant method by requiring that the decimation functions asymptotically converge to a period p limit cycle. In particular, we used $f_n(0) = f_{n-p}(0)$ with e.g. $n = 17, 20, 23$, where the cantorus was approximated with an orbit of the length $F_{23}=46368$. Table I compares E_{min} obtained in this way at $k = 2$ with diagonalization results. One should note that the above self-consistent calculation of E_{min} is not only more accurate but also takes only a small fraction of the CPU time needed for the diagonalization of a matrix of the size $10946/2$. All the computations were done using quadruple precision.

The critical line for the one to two-hole transition was determined by the symmetry breaking bifurcations as in ref. [10]. Table II lists the bifurcation points of periodic orbits along the line $k_2 = 4k_1$. It can be seen in this table that due to superexponential convergence, all decimals of the quadruple precision are already exhausted at the orbit length 377. This size is highly inadequate because it limits the maximum number of decimation iterations to be 14. With 14 iterations, we are still in the transient regime and the existence of a limit cycle for the decimation functions is far from obvious. Moreover, the nature

of phason eigenfunction or the fate of the orbit Lyapunov exponent cannot be decided on such a short orbit. To overcome this problem, we used a multi-precision software package [11] to compute the orbit and the phonon eigenfunction along the one to two-hole transition line (see Section VI for further details).

V. RENORMALIZATION BIFURCATION DIAGRAM

The two-step numerical procedure discussed in the previous section was applied to study the scaling properties of the phonon eigenfunctions for a multitude of values of k starting from the KAM phase upto the *anti-integrable limit* $k \rightarrow \infty$. This limit corresponds to vanishing elastic interaction [5] which implies that for a m.e. state all balls lie at the potential energy minimum $x = 1/2$. By introducing the parameter $r = 2 \arctan(k)/\pi$ one can map the whole k -axis to the r -interval $[0, 1]$, where $r = 0$ and $r = 1$ are the integrable and anti-integrable limits, respectively.

In the KAM region, where the invariant circle is smooth, one obtains the same trivial fixed point for all classes of approximating orbits. It can be easily solved from the fixed point equation: $f_n(i) \equiv \sigma$ and $e_n(i) \equiv -\sigma^2$. It describes an extended quasiperiodic phonon eigenfunction.

In general, choosing the class fixes the phase ϕ in Eq. (6) and thus different classes can lead to different decimation cycles. This is the case at the TBA, where the class 1 and 3 orbits having x_0 on the dominant symmetry line lead to a nontrivial universal fixed point [17] whereas the class 2 and 4 orbits correspond to 3-cycles. In Fig. 1 we plot the critical phason ($\omega = 0$) mode ψ_i obtained by approximating the invariant circle by the class 1 or 3 orbits which causes the main peak to be located at $i = 0$. The non-trivial fixed point and the corresponding self-similarity clearly distinguishes the TBA from the KAM regime.

In the cantorus regime, both classes 2 and 4 lead to the same decimation 6-cycle for fixed k . Fig. 2(a) shows the variation of the 6-cycle as we change the parameter r from the KAM region to the anti-integrable limit. An interesting feature of the diagram is the infinite number of *loops* separated by *degeneracy points* where the decimation functions approach asymptotically the same trivial limit cycle as in the KAM phase. Coming down from the anti-integrable limit, the first such degeneracy is found at $r = 0.67052674\dots$. Although the decimation functions come close to the trivial fixed point already near $r = 0.84$, they behave parabolically in this region forming an avoided crossing. As shown in the blowup of Fig. 2(b), the behaviour is very different around $r = 0.67052674$ where the curves behave linearly as a function of the parameter r all passing through the inverse golden mean

at the same point. Table III gives a list of degeneracy points. We have checked that they all correspond to a real crossing of the curves in the bifurcation diagram. We conjecture that there are an infinite number of such points accumulating at the critical parameter value for the TBA.

As can be seen in Table III, the separation between subsequent degeneracy points appear to asymptotically scale by the universal scaling constant $\delta = 1.62795\dots$ for the TBA [21,22]. This suggests that the observed loop pattern is related to the renormalization dynamics along the unstable manifold of the TBA fixed point. This in turn causes one to think that there should be some property of the configurations which makes the degeneracy points special. If such a property exists, it has to be rather subtle as the orbit hull function is given by qualitatively the same kind of series of step functions through the whole cantorus region.

An important property associated with the degeneracy points is revealed by plotting the *phonon hull*, i.e. ψ_i versus $\{i\sigma\}$ where $\{i\sigma\}$ is the fractional part of $i\sigma$. Fig. 3(a) shows this plot at one of the degeneracy points. The resulting graph appears to be represented by an infinite series of step functions. Similar plots are obtained at other degeneracy points. In other words, the phonon hull shows similar characteristics as the orbit hull function g at these points. It is interesting to note that this is not only true at the degeneracy points but also in the KAM phase where both the orbit and phonon hull functions are smooth. This suggests that trivial asymptotic decimation functions in general signify qualitatively equivalent behavior in the quasiperiodic “potential” term of the linear difference equation and in the corresponding (generalized) eigenfunction.

In the cantorus regime outside the degeneracy points, the phonon hull consists of a fractal set of points resembling the phonon hull function at the TBA. Fig. 3(b) shows how the character of the phonon hull changes as we move away from the degeneracy points. The existence of a decimation limit cycle implies self-similarity of the phonon eigenfunction. This self-similarity is clearly seen after adjusting the phase factor so that the eigenfunctions remain bounded asymptotically [3]. Interestingly, the resulting decimation trajectories converge on a 4-cycle. The 4-cycle appears to be more fundamental (and interesting because it breaks the number theoretic even-odd 3-cycle) than the 6-cycle. It means there is a point on the cantorus around which the phonon mode is self-similar although none of the approximating orbits pass through it. However, since the qualitative features of the bifurcation diagram (loops and degeneracy points) are similar using the 4 or 6-cycle, for simplicity, our bifurcation diagrams are shown with 6-cycle.

VI. TWO-HARMONIC MODEL AND THE ONE TO TWO-HOLE TRANSITION

Next we study the phonons and the associated renormalization bifurcation diagram in the two-harmonic FK model with potential

$$V(x) = \frac{k_1}{4\pi^2} \cos(2\pi x) + \frac{k_2}{16\pi^2} \cos(4\pi x). \quad (13)$$

Our motivation for this study is two-fold: firstly, to see if loops and degeneracy points are generic in such models and secondly, to obtain the renormalization bifurcation diagram near the one to two-hole transition for cantori studied recently by Baesens and MacKay [10].

As stated in their paper, a *gap* in a cantorus is a pair of distinct points of the cantorus whose forward and backward orbits converge together. An orbit of gaps is called a *hole*. In the standard map with single well potential, the cantorus is uniquely determined by the rotation number (if there is no invariant circle with that rotation number) and contains only one hole. However, in the two-harmonic model the cantori for a given rotation number are parametrized by $\alpha \in [0, 1]$ near a non-degenerate double-well anti-integrable limit with $|k_1| < |k_2|$ [9]. Here α gives the fraction of the natural measure of the cantorus in one of the wells. In other words, there are uncountably many cantori of each rotation number. They have generically two holes although there is a dense set of values of α corresponding to only one hole. Using symmetry properties it can be argued for $k_2 > 0$ that the m.e. cantorus has an equal fraction of points at both wells near the anti-integrable limit [9]. Thus Baesens and MacKay [10] focus on $\alpha = 1/2$. Numerically they observe a critical line in the $k_1 - k_2$ parameter space corresponding to the one to two-hole transition for the symmetric cantorus with $E_{min} = 0$.

Fig. 4(a) shows the renormalization bifurcation diagram obtained by varying the parameter

$$r = \frac{2}{\pi} \arctan \sqrt{k_1^2 + k_2^2} \quad (14)$$

along the line $k_2 = 4k_1$. We followed the same numerical methods as in the previous section and approximated the cantorus by class-2 orbits (the class-4 orbits give a homoclinic in addition to the cantorus in the region of two holes). The figure clearly shows the existence of loops and degeneracy points near the TBA thus establishing the result that their existence is generic in one-parameter systems.

The transition from one to two holes is signalled by a divergence in one of the six members of the limit cycle. The other members of the limit cycle are found to remain finite. Furthermore, the bifurcation diagram in the neighborhood of the one to two-hole transition exhibit a rather strange pattern due to the fact that various members of the limit cycle cross each other as the parameter r

is varied. However, the limit cycle retains the period six at these crossing points. The crossing pattern becomes more and more complicated near the 1-2 hole transition. There can be a multitude of crossings in a very narrow parameter interval which makes the behaviour of the curves look discontinuous at some points. However, blowups reveal that the curves are in fact smooth (see Fig. 4(b)).

We have also studied the critical line corresponding to the hole transition in the $k_1 - k_2$ space. Our numerical results strengthen the previous conjecture [10] that the Lyapunov exponent of the extended standard map vanishes along the hole transition (see Table IV). The decimation functions obtained with class 2 orbits converge on a 6-cycle with one member of the cycle diverging while the remaining elements of the 6-cycle remain bounded and vary continuously along the transition line. Numerically the phason mode is found to be peaked around the lattice site i_c corresponding to x_{i_c} which is closest to $1/2$. Therefore, on the transition line it is natural to look at class-4 orbits because they have the 0th point exactly at $1/2$. However, we find no non-trivial limit cycle with the class-4 orbits reflecting the fact that the phason mode vanishes asymptotically as $i \rightarrow \pm\infty$. This localization is non-exponential with the inverse localization length $\gamma = 0$. In Fig. 5 we plot the phason mode in both linear-log and log-log scales. These plots show that the localization is slower than exponential but faster than geometric. To our knowledge, this peculiar behaviour of the eigenfunctions has not been observed before.

Another unique aspect of the two-harmonic model is the fact that it is possible to show the existence of critical phonon modes in the anti-integrable limit. This is clearly seen in Fig. 4(a) where the phonon eigenfunctions are characterized by a non-trivial limit cycle even approaching $r = 1$. As explained in Appendix, for a generic symmetric two-well potential the universality class in the anti-integrable limit is determined by σ , α , and two additional parameters setting the location of the minima and the ratio of the third and second derivative of the potential at the minima. For the potential (13) the latter two parameters are both fixed by the ratio k_2/k_1 .

VII. DISCUSSION

Based on exact renormalization methods which can be implemented to very high precision on the computer, we have shown that the phonon eigenfunction at the minimal frequency is self-similar with scaling properties that vary continuously within the cantorus regime. A novel feature of our study is the existence of a sequence of points where the phonon eigenfunctions are represented by series of step functions. An important aspect of the work described here is the new method to compute eigenvalues. The determination of the bifurcation diagram near the TBA was a challenging numerical problem and

would have been impossible without the self-consistent approach provided by the decimation scheme.

It is interesting to compare our results with those for a related electron problem [19,20]. The TBA in the FK model is somewhat analogous to the metal-insulator transition for two-dimensional electrons due to the formal similarity between the phonon equation and the corresponding equation for the electron wave functions. However, the innocent looking difference in the quasiperiodic potential leads to significantly different behaviour beyond the transition. In the “insulating” phase of the electron problem, the wave functions are exponentially decaying with self-similar fluctuations characterized by a unique renormalization fixed point. In contrast, the phonon eigenfunctions in the cantorus regime exhibit self-similarity without exponentially decaying envelope and can be described by a line of renormalization limit cycles. Furthermore, the cantorus phase contains an infinite number of special points where the renormalization flow converges to the same trivial fixed point as in the KAM phase or in the “metallic” phase of the electron problem. The anti-integrable limit is trivial for the standard FK model but non-trivial in the region of a two-hole cantorus. In comparison, the counterpart of the anti-integrable limit in the electron problem, the strong coupling limit is always highly nontrivial.

The above described degeneracy points remain one of the main mysteries of our discoveries. In particular, why do the degeneracy points appear in the cantorus phase starting arbitrarily close to the TBA and why do they disappear beyond a certain value of the nonlinearity parameter? We have tried to correlate them with some special characteristics of the ball configurations of the FK model but without success. Furthermore, the complexity of the renormalization flow near the one to two-hole transition is very puzzling and devoids of any explanation.

Our results have significance in the theory of an almost periodic eigenvalue problem. Degeneracy points are the first example in this class of problems whose solutions can be represented by an infinite series of step functions. Another curious feature are the non-exponentially decaying eigenfunctions at the one to two-hole transition in an extended FK model.

In this paper, we have explored only the parameter region $k_2 > 0$ of the extended FK model. However, there is a really rich pattern of cantorus bifurcations for $k_2 < 0$ [9,18]. In particular, Schellnhuber et al. [24] have reported exponential localization of the phason mode at a boundary of metastability in an extended version of the FK model containing three harmonics. The metastability is related to vanishing of the gap of the phonon spectrum which in that case signals annihilation of the cantorus configuration. It would be interesting to apply the decimation method at this and other similar bifurcations and determine the scaling properties of the exponentially localized eigenfunctions.

One of the most intriguing features of studying the phonons in the FK model is that various different subjects like condensed matter physics, nonlinear dynamics, almost periodic Schrödinger operators, and renormalization theory are drawn together. We hope that the results of this paper motivate further research in each of these fields.

ACKNOWLEDGMENTS

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APPENDIX: PHONONS IN THE ANTI-INTEGRABLE LIMIT

Here we explain the origin of the non-trivial critical behavior of the phonons for the double-well anti-integrable limit (AIL). This will account for the differences at $r = 1$ in Fig. 2(a) and the Fig. 4(a). In particular, we derive an equation for the critical phonons corresponding to a two-hole cantorus approaching the AIL.

The key point of the derivation is the fact that the limiting form of the potential seen by the phonons approaching the AIL is determined not by the locations of the balls at the AIL (which gives a constant contribution) but by the small deviation in the ball positions from those at the AIL.

It is useful to multiply the phonon equation (8) by the factor

$$t = \frac{1}{\sqrt{k_1^2 + k_2^2}} \quad (\text{A1})$$

so that all terms in the equation remain bounded in the AIL $t \rightarrow 0$:

$$t\psi_{i+1} + t\psi_{i-1} - [2t + U''(x_i)]\psi_i = -\bar{\omega}^2\psi_i, \quad (\text{A2})$$

where $U(x) = tV(x)$ and $\bar{\omega}^2 = t\omega^2$. It is important that U does not depend on the value of t if the ratio k_2/k_1 is fixed. We now expand $U(x)$ around the ball position at the AIL which we denote as e_i . Since $U'(e_i) = 0$, we have

$$U'(x_i) = U''(e_i)\xi_i + O(\xi_i^2), \quad (\text{A3})$$

where $\xi_i = (x_i - e_i)$ is the small deviation in the ball configuration from that of the AIL. Using the equation

$$U'(x_i) = t(x_{i+1} - 2x_i + x_{i-1}) \quad (\text{A4})$$

we notice that ξ_i changes linearly with t near the AIL. Therefore, upto the first order in t , we have

$$\xi_i = \frac{td_i}{U''(e_i)}, \quad (\text{A5})$$

where $d_i = e_{i+1} - 2e_i + e_{i-1}$. The next step is to put this together with the expansion

$$U''(x_i) = U''(e_i) + U'''(e_i)\xi_i + O(\xi_i^2) \quad (\text{A6})$$

into Eq. (A2). Because $U''(e_i)$ is equal for all i if $k_2 > 0$, it is possible to match the zeroth and first order terms in t so that one obtains the asymptotic equation

$$\psi_{i+1} + \psi_{i-1} + V_{AIL}(i)\psi_i = (2 + C)\psi_i, \quad (\text{A7})$$

where C is the limit of $-\omega^2 + U''(e_i)/t$ as $t \rightarrow 0$ and

$$V_{AIL}(i) = -\frac{U'''(e_i)d_i}{U''(e_i)}. \quad (\text{A8})$$

In the case of a single well, the potential is even around the minimum and the resulting asymptotic phonon equation becomes simply

$$\psi_{i+1} + \psi_{i-1} = (2 + C)\psi_i. \quad (\text{A9})$$

E_{min} corresponds to the supremum of the spectrum which in this case is 2, i.e. $C = 0$.

In the case of two wells for $|k_1| < k_2$ a straightforward calculation shows that

$$\frac{U'''(e_i)}{U''(e_i)} = \pm \frac{6\pi}{\sqrt{(k_2/k_1)^2 - 1}}, \quad (\text{A10})$$

where the $+$ ($-$) sign corresponds to $\{e_i\} > 1/2$ ($\{e_i\} < 1/2$). Let us next study the possible values of d_i assuming that $\sigma = (3 - \sqrt{5})/2$. The hull function which gives the set e_i at the AIL reads [9,10]

$$g_e(\theta) = \begin{cases} x_m + \text{Int}(\theta), 0 < \{\theta\} < \alpha \\ 1 - x_m + \text{Int}(\theta), \alpha < \{\theta\} < 1 \end{cases}, \quad (\text{A11})$$

where x_m is the minimum in $(0, 1/2)$ satisfying $\cos(2\pi x_m) = -k_1/k_2$. In the symmetric case $\alpha = 1/2$ it is easy to see that d_i can have only the values

$$d_i = \begin{cases} \pm 2x_m, \theta_i \in \{(0, 1/2 - \sigma), (1/2 + \sigma, 1)\} \\ \pm(4x_m - 1), \theta_i \in \{(1/2 - \sigma, \sigma), (1 - \sigma, 1/2 + \sigma)\} \\ \pm(2x_m - 1), \theta_i \in (\sigma, 1 - \sigma) \end{cases}, \quad (\text{A12})$$

where $\theta_i = i\sigma + \phi$ and the \pm sign cancels the one coming from Eq. (A10). Because the potential V_{AIL} takes only three different values, the generalized eigenfunctions cannot be localized [14]. E_{min} corresponds to the supremum of the spectrum of Eq. (A7). The class 2 orbit corresponds to choosing the phase $\phi = -\sigma/2$ in the hull

function [10]. Decimation with this phase leads to the non-trivial 6-cycle found by extrapolating the curves of a bifurcation diagram to the AIL.

It is interesting to note that V_{AIL} is determined solely by σ , α , x_m , and a multiplying factor. Therefore, other similar two-well potentials for which these parameter agree would give rise to the same universality class in the AIL.

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- [1] e-mail: isatija@sitar.gmu.edu.
 - [2] If the decimation was carried for ψ_i , the inverse localization length would be determined by the decay rate of e_n , i.e. $\gamma = \lim_{n \rightarrow \infty} \ln(e_n(0))/F_n$.
 - [3] Although the inverse localization length γ is zero, the phonon eigenfunctions corresponding to the nontrivial 6-cycles diverge very slowly as $i \rightarrow \pm\infty$ at other than the Fibonacci sites. There are general results on almost periodic Mathieu operators [25] which claim the existence of a critical phase ϕ_c for which the generalized eigenfunction should be bounded. Numerically we find the point $x_c = g(\phi_c)$ on the cantor by monitoring the largest peak of the phonon mode in a finite region $-F_n < i < F_n$. Assuming it takes place at the lattice site $i(n)$, x_c can be approximated by $x_{i(n)}$. Increasing n we can get arbitrarily close to x_c and using lattice translations we can carry out the decimation with $x_0 \approx x_c$. The eigenfunction is not symmetric around this point. See ref. [19] for analogous results on the electron tight binding model.
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FIG. 1. Universal phason mode at the TBA with $x_0 = 0$.

FIG. 2. (a) Renormalization bifurcation diagram showing the asymptotic behaviour of the decimation function f as a function of the parameter $r = 2\arctan(k)/\pi$. At each parameter value, $f_n(0)$ is plotted for at least $(p+2)$ different decimation levels n which shows the accuracy of the limit cycle (of length p) obtained. The 3-cycle at the TBA is plotted with darker points. The curves behave parabolically near $r = 0.84$ and do not intersect there. (b) Blowup around the first degeneracy point where the branches of the 6-cycle meet at an intersection point.

FIG. 3. Phonon hull at the second degeneracy point $r = 0.62221\dots$ (a) and away from it at $r = 0.62$ (b).

FIG. 4. Renormalization bifurcation diagram for the extended FK-model with $k_2 = 4k_1$. (a) shows the elements of the limit cycle that remain bounded by 2 near the one to two-hole transition and (b) shows an example of how complicatedly the curves can cross one another in a very narrow parameter interval. For an analogous configuration bifurcation diagram see Fig. 1 of ref. 10.

FIG. 5. Phason eigenfunction with $x_0 = 1/2$ at the one to two-hole transition plotted in linear-log (a) and log-log (b) scales. These plots show that the localization is between exponential and power-law.

TABLE I. Estimates for the infimum of the phonon spectrum E_{min} at $k = 2$. The values in the third column were obtained by diagonalizing a matrix of size $F_n/2$ as described in ref. 10. The values in the last column were determined by requiring that $f_n(0) = f_{n-6}(0)$ where the sequence x_i was approximated by the class-2 orbit of the length 46368.

n	F_n	E_{min} (diag.)	E_{min} (dec.)
14	610	0.5935392137880	0.5935394324321
17	2584	0.5935394985221	0.5935394834426
20	10946	0.5935394812326	0.5935394820297
23	46368		0.5935394820545

TABLE II. Symmetry breaking bifurcations of class 4 orbits along the line $k_2 = 4k_1$. The bifurcation points have been calculated using multiprecision software based on doubly precision arithmetics. We have checked consistence with a direct calculation using quadruple precision. The bifurcation points converge fast to the critical parameter value for the one to two-hole transition. Note that the corresponding value 0.429439737992501223898752836653609 obtained in ref. 10 appears to be accurate only upto double precision.

F_n	k_1
377	0.4294397379925012239000251474523975392588953 5245566429536,
987	0.4294397379925012239000251474523975392588953 7931282057125515563523777678 714122115567680849012510667905,
1597	0.4294397379925012239000251474523975392588953 7931282057125515563523777678 9131402934114670775341029280082904661719,

TABLE III. Degeneracy points approaching the critical parameter value r_c from above and their scaling.

n	r_n	$(r_{n-1} - r_c)/(r_n - r_c)$
0	1.00000000	
1	0.67052674	2.8336
2	0.62221221	1.3678
3	0.56379391	1.8008
4	0.53923590	1.5075
5	0.51909955	1.7126
6	0.50876597	1.5765
7	0.50162025	1.6630
8	0.49754645	1.6076

TABLE IV. Lyapunov exponent λ of the F_{n-2}/F_n orbit (class 2) at the one to two-hole transition point with $k_2 = 4k_1$. The transition point was approximated by the last parameter value in Table II. The symmetry breaking points of the odd cycles converge faster than those of the even cycles which justifies the inclusion of the Lyapunov exponent of the 2584-orbit in this table.

F_n	λ
34	0.38572449
144	0.20463797
610	0.10618378
2584	0.05450141

Fig1 Ketoja and Satija

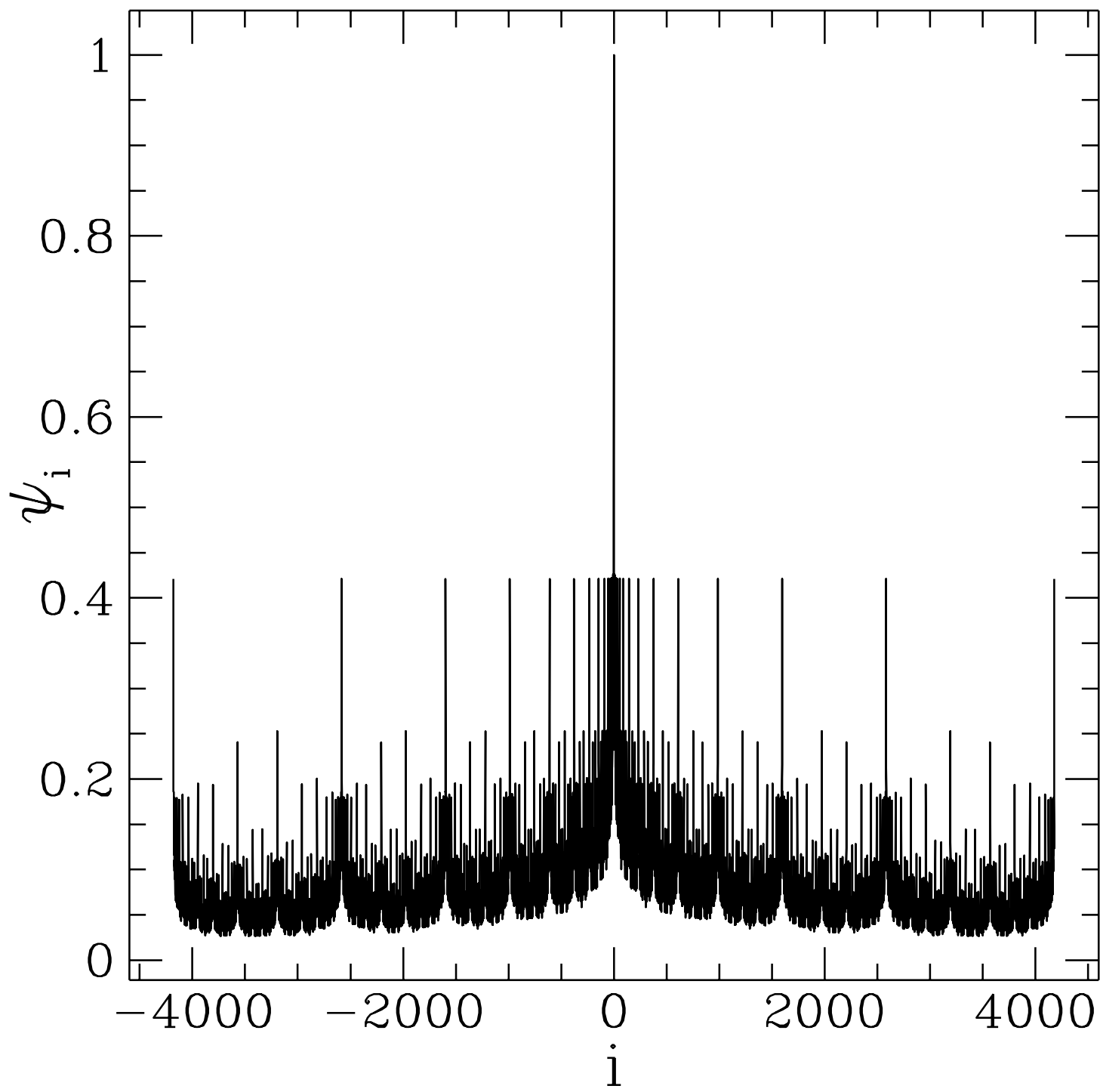


Fig2 Ketoja and Satija

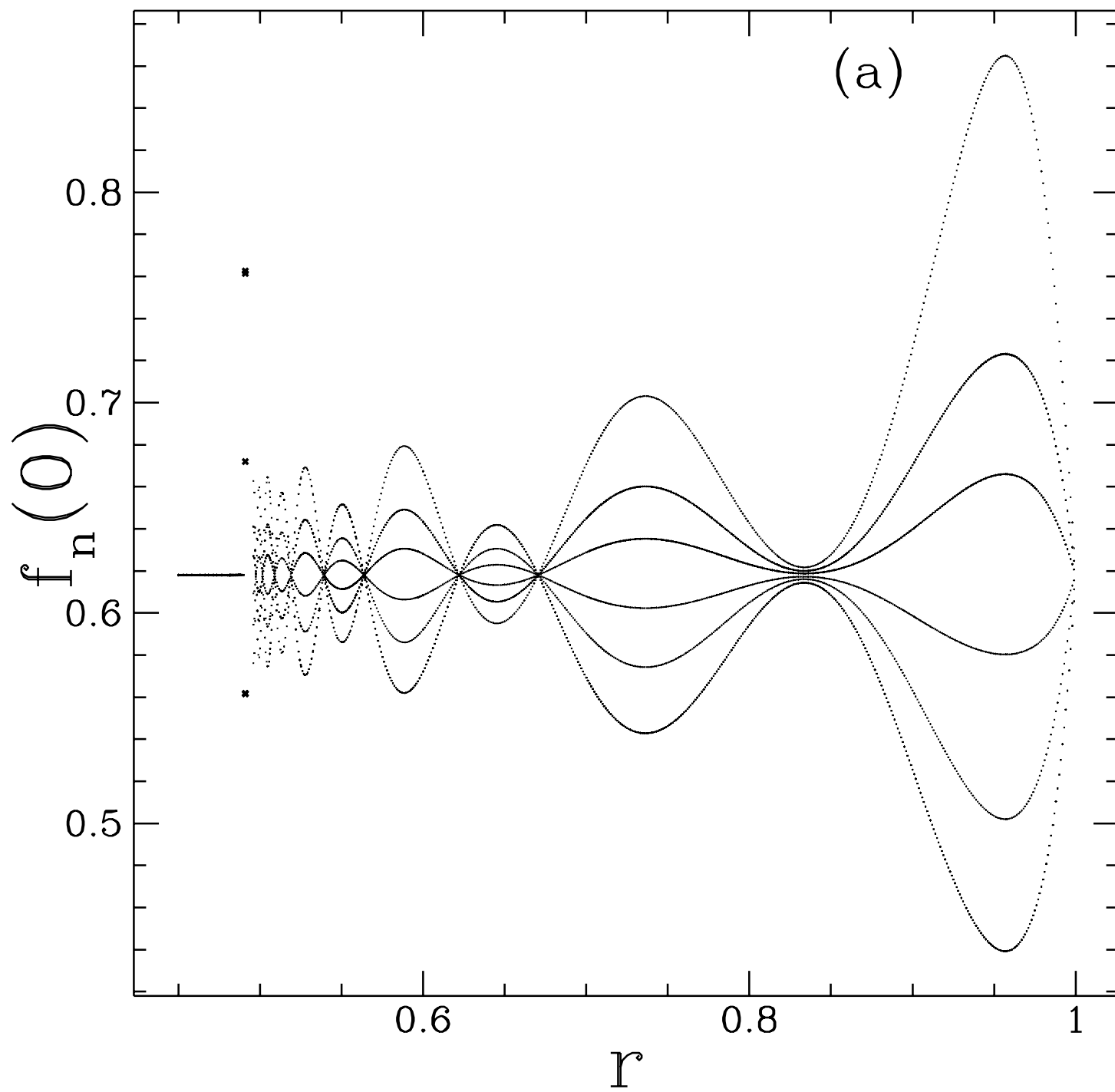


Fig2 Ketoja and Satija

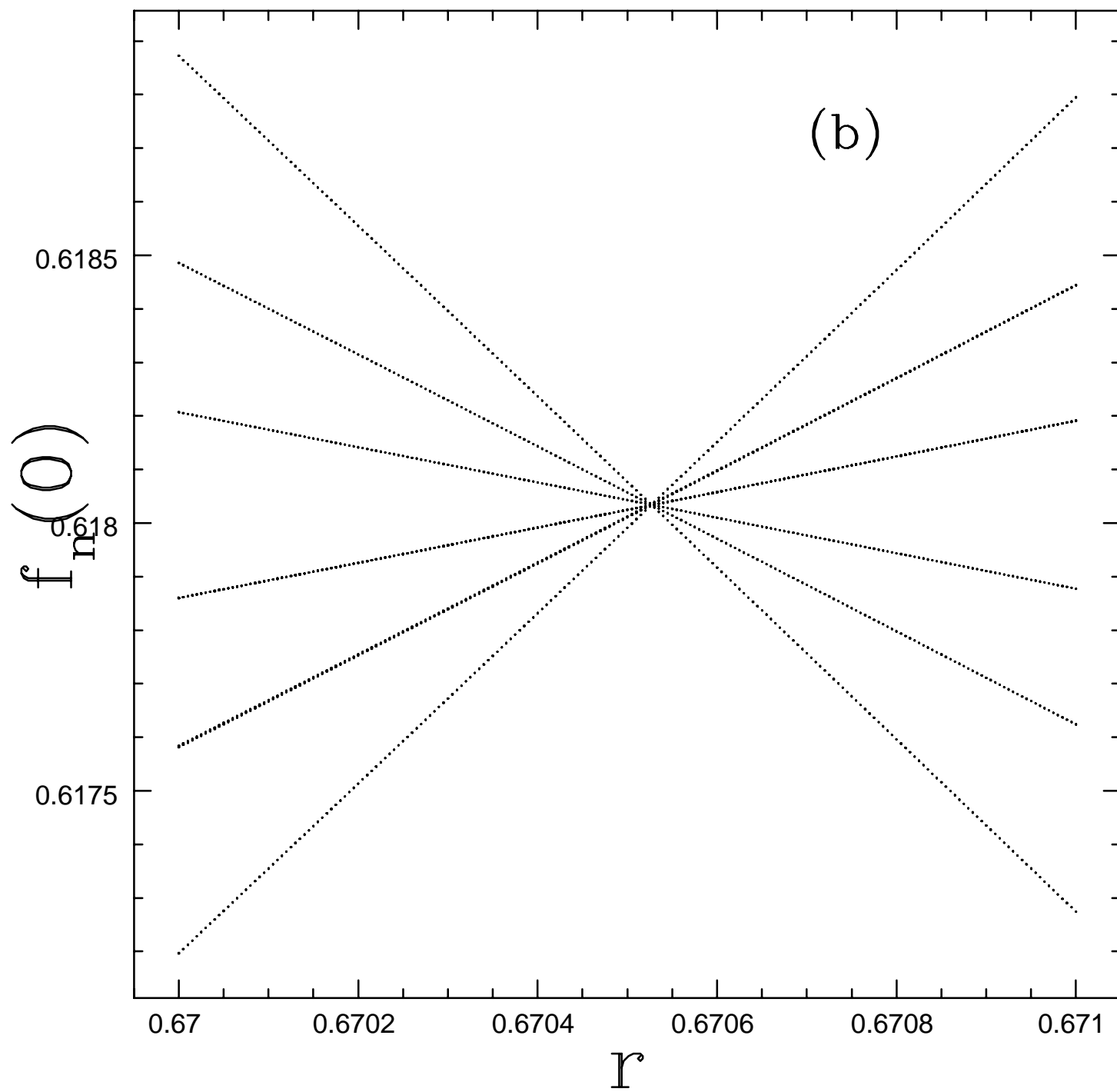


Fig3 Ketoja and Satija

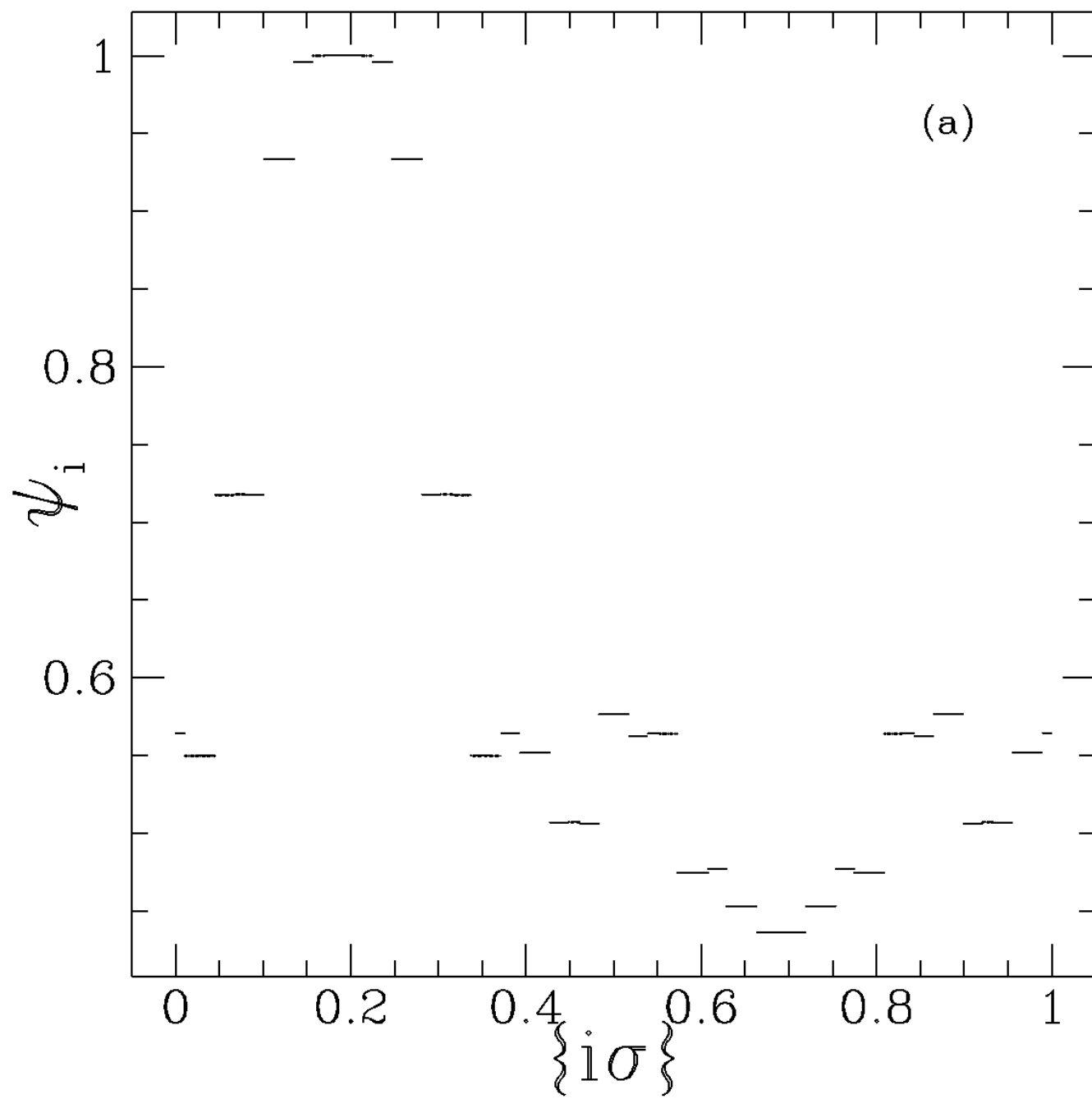


Fig3 Ketoja and Satija

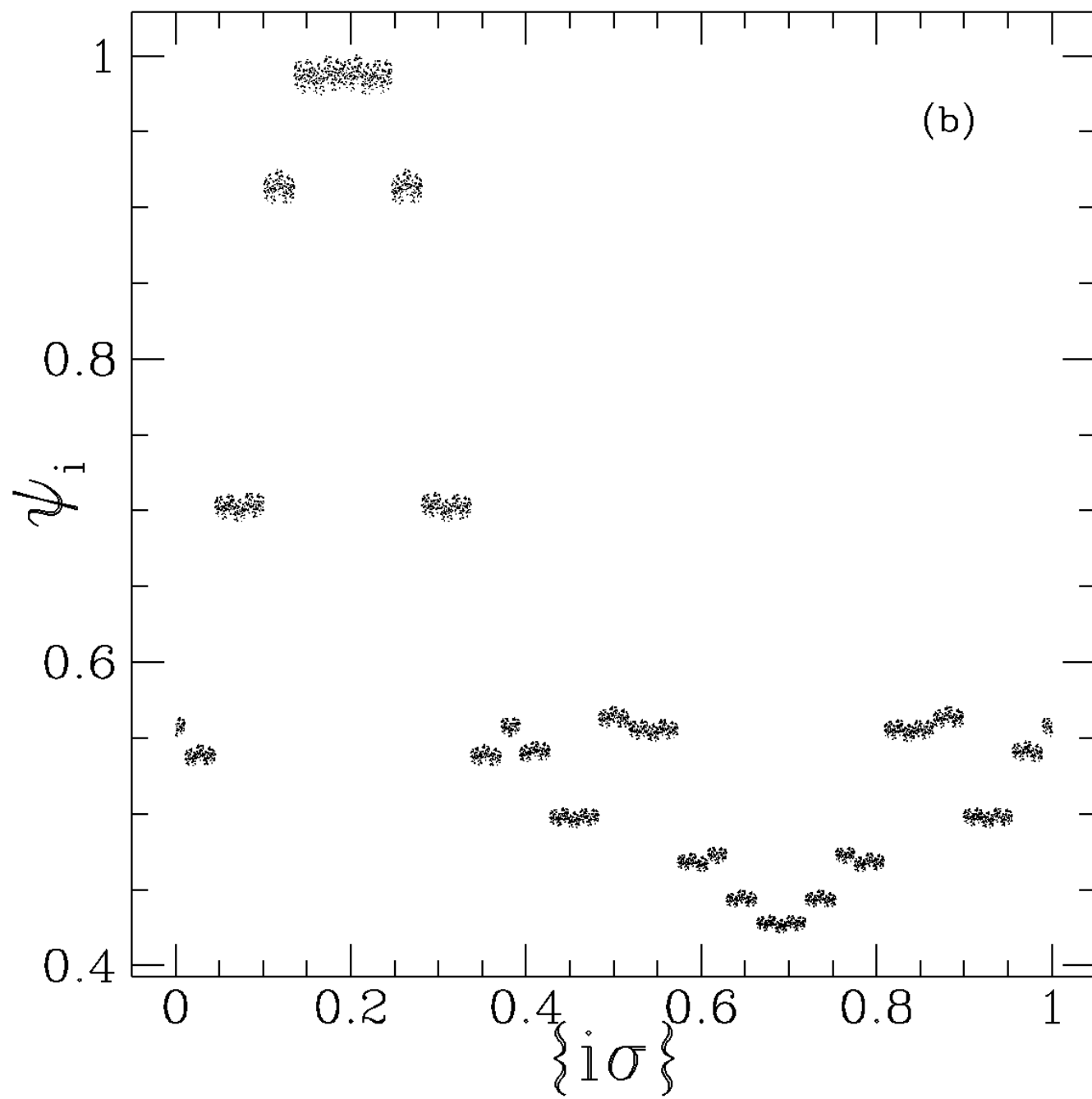


Fig4 Ketoja and Satija

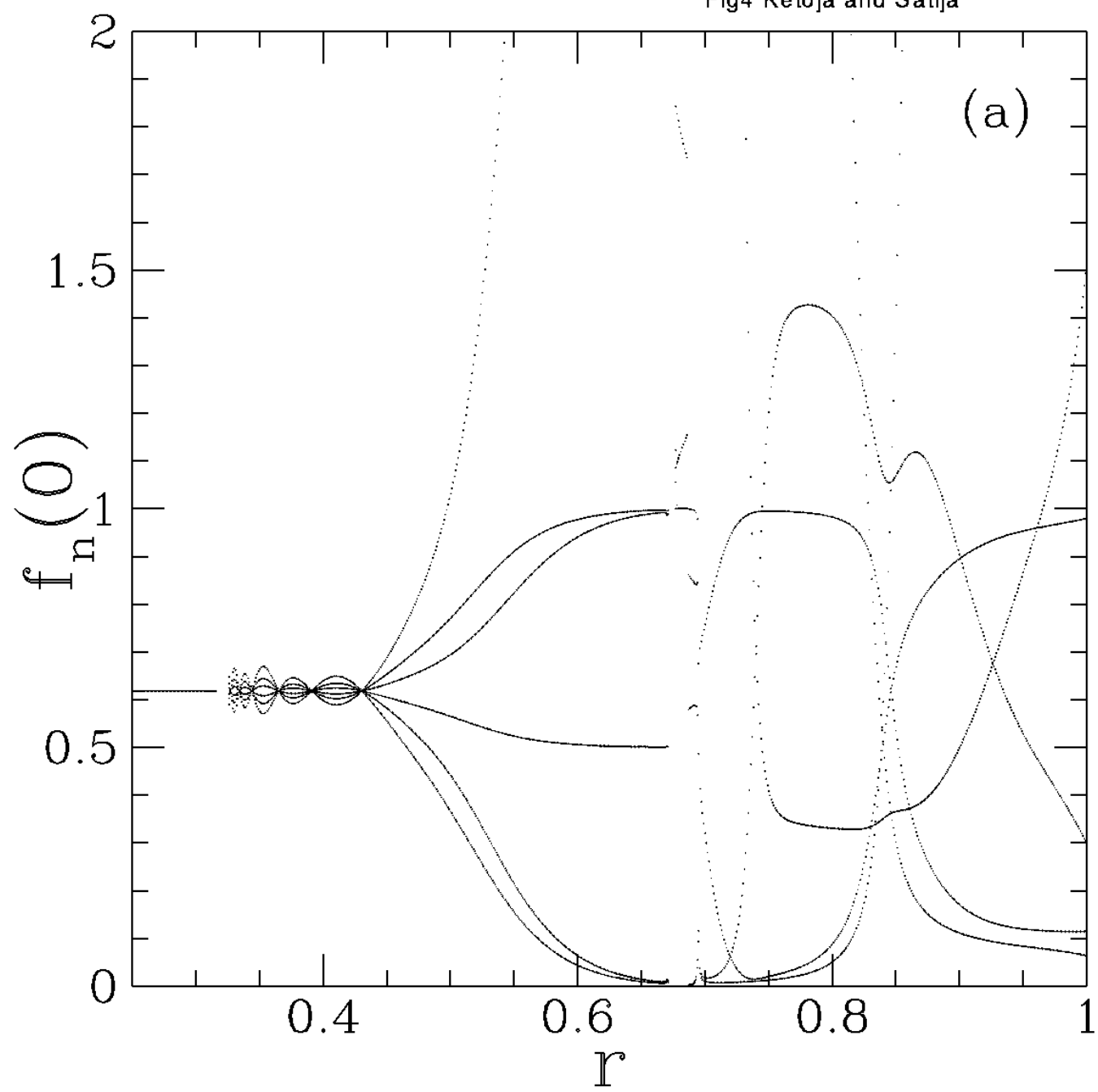


Fig4 Ketoja and Satija

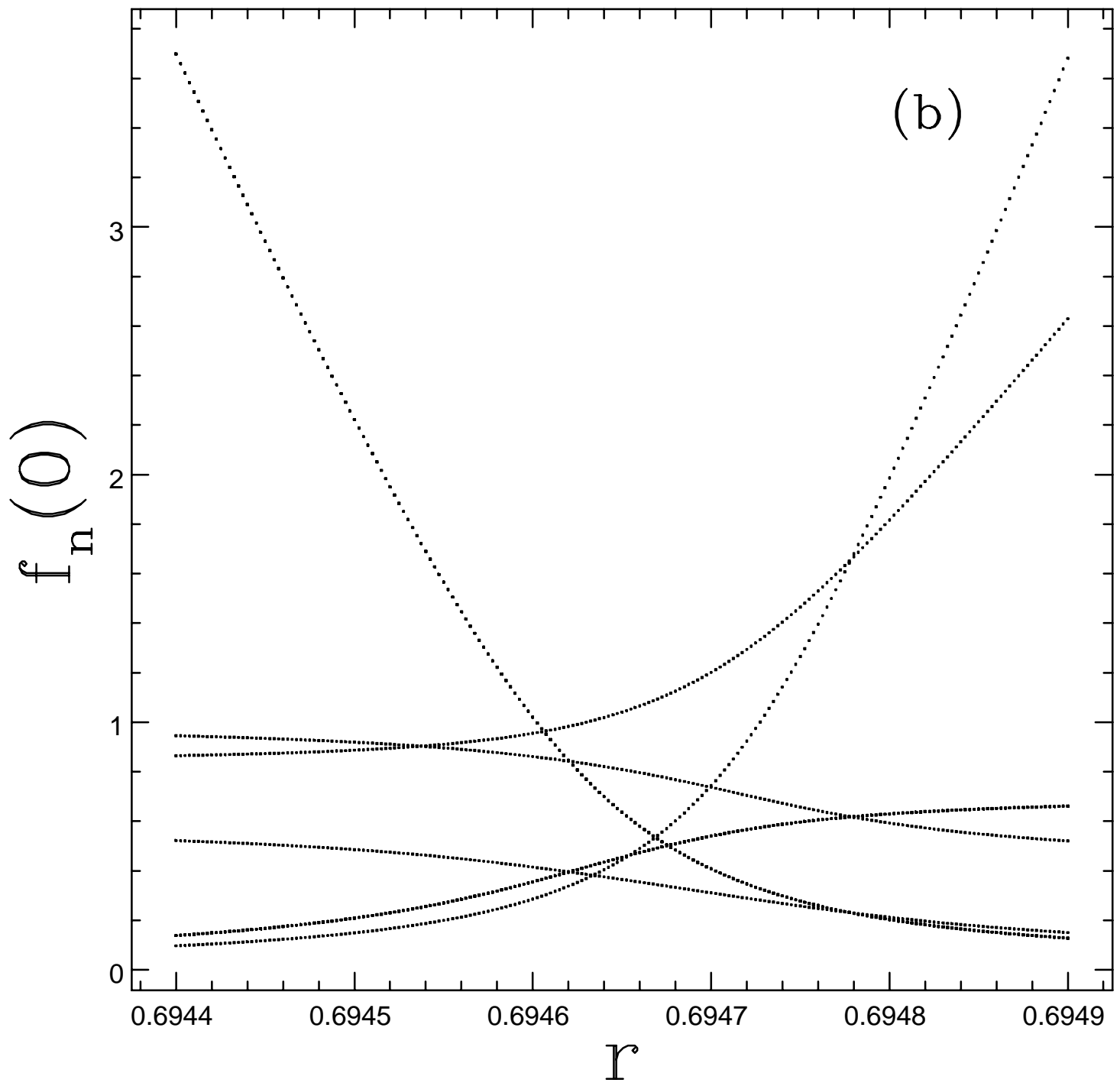


Fig5 Ketoja and Satija

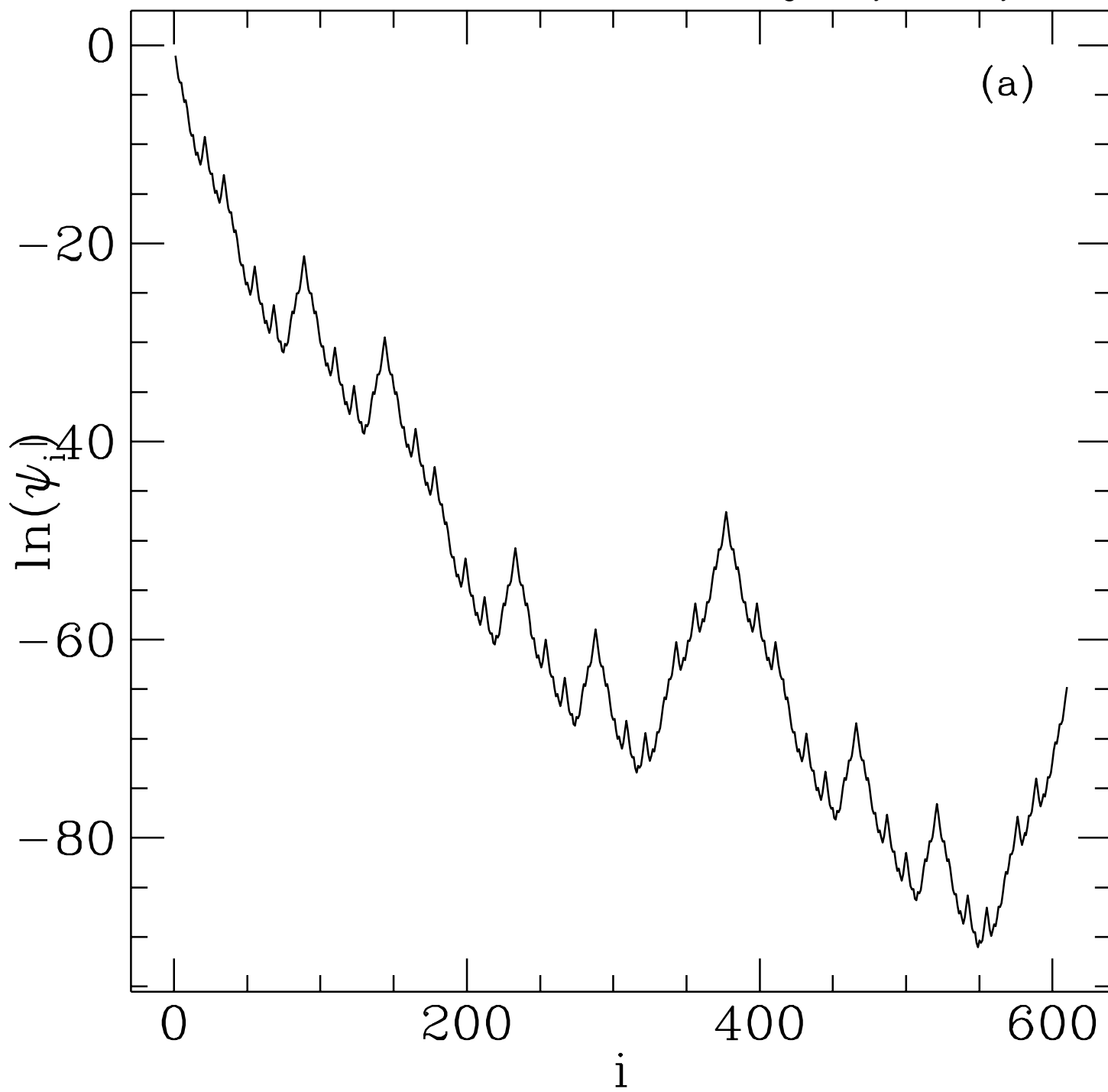


Fig5 Ketoja and Satija

